DSMC Convergence Behavior for Fourier Flow

D. J. Rader[1], M. A. Gallis[1], J. R. Torczynski[1], and W. Wagner[2]

[1]*Engineering Sciences Center; Sandia National Laboratories; Albuquerque, New Mexico 87185-0834 USA*
[2]*Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstrasse 39, D-10117, Berlin, Germany*

Abstract. The convergence behavior of Bird's Direct Simulation Monte Carlo (DSMC) method is explored for near-continuum, one-dimensional Fourier flow. An argon-like, hard-sphere gas is confined between two parallel, fully accommodating, motionless walls of unequal temperature. The simulations are performed using a one-dimensional code based on Bird's DSMC prescription. The convergence metric is taken as the ratio of the DSMC-calculated bulk thermal conductivity to the infinite-approximation, Chapman-Enskog (CE) theoretical value. The convergence rate is monitored with respect to three parameters: time step, cell size, and number of computational molecules per cell. For a sufficiently large number of computational molecules, the DSMC discretization error is observed to decrease quadratically with time step and cell size, in good agreement with previous predictions based on Green-Kubo theory. When all three parameters are finite, the observed convergence behavior is complex. As numerical errors are systematically reduced, the DSMC-calculated conductivity is shown to approach the theoretical CE value to within 0.02%, showing that the present implementation of Bird's DSMC algorithm provides an excellent representation of continuum, CE heat conduction.

INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method employs a particle-based, stochastic algorithm to solve the Boltzmann equation by approximating the continuous molecular velocity distribution function with a discrete set of computational molecules [1]. Historically, DSMC has been very successful in the study of rarefied, high-speed flows typical of aerospace engineering [1,2]. The validity of the method for this class of problems has been firmly established by comparisons to experimental data [3] and molecular-dynamics calculations [4]. More recently, the DSMC method has become increasingly popular as a means for exploring ambient-pressure flows in nano- and micro-scale geometries, such as are found in thin-film bearings [5], oscillating microbeams [6], and microchannels [7,8]. Often, these small-scale systems involve near-continuum and/or low-speed flows that are challenging to simulate with stochastic algorithms. For example, one DSMC study of ambient-pressure, low-speed (~1 m/s) micro-Couette flow suggests that statistical errors become large enough to preclude accurate simulations [8]. Near-continuum DSMC studies of the motionless-gas Fourier problem have been more successful. For example, several studies report DSMC simulations that give bulk thermal conductivities that agree with Chapman-Enskog (CE) theoretical predictions to within ~10% [9,10]. These authors note that some of the observed deviations may arise from the finite nature of the computational domain. Recently, Gallis et al. [11] performed very careful DSMC simulations of the Fourier problem and found excellent agreement (~0.2%) between their calculated bulk thermal conductivity and the CE infinite-approximation result. They also showed that the DSMC-calculated velocity distribution function, as measured by the Sonine-polynomial coefficients a_k, was in excellent agreement with CE theoretical predictions [12]. Thus, at least for the Fourier problem, it appears that careful applications of the DSMC method can provide solutions that are in good agreement with the CE approximation to the Boltzmann equation.

One drawback to achieving high-accuracy solutions with the DSMC method is the high computational burden. Consequently, a clear understanding of how to achieve a specified level of numerical accuracy with a minimum of computational effort is needed. In response, this paper provides a convergence study of the DSMC method for the one-dimensional Fourier heat-flow problem. The convergence metric is taken as the ratio of the DSMC-calculated bulk thermal conductivity, K_{DSMC} to the infinite-approximation, CE theoretical value, K [11,12]. To ensure that the CE

CP762, *Rarefied Gas Dynamics: 24th International Symposium,* edited by M. Capitelli

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED
13 JUL 2005	**N/A**	**-**

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
DSMC Convergence Behavior for Fourier Flow	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Engineering Sciences Center; Sandia National Laboratories; Albuquerque, New Mexico 87185-0834 USA**	8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001792, International Symposium on Rarefied Gas Dynamics (24th) Held in Monopoli (Bari), Italy on 10-16 July 2004.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			
unclassified	**unclassified**	**unclassified**	**UU**	**6**	

limit is achieved, DSMC simulations are performed for a small system Knudsen number (~0.02) and with a modest temperature gradient (100 K/mm). These conditions lead to solutions for which the normal solution in the central region of the domain can be clearly differentiated from the Knudsen layers near each wall. Four parameters are known to limit the numerical accuracy of the DSMC method: the number of independent samples per cell, M_c; the number of simulators (particles) per cell, N_c; the time step, Δt; and the cell size, Δx. The present calculations employ large enough samples such that statistical errors are reduced to levels that are negligible compared to the contributions of the other three parameters. The remaining, non-statistical error (herein referred to as the discretization error) is systematically explored as a function of N_c, Δt, and Δx.

FOURIER PROBLEM

The Fourier problem consists of one-dimensional heat flow through a hard-sphere gas confined between two parallel, fully accommodating, motionless walls of unequal temperature. The wall at $x = 0$ is held at a lower temperature, T_C, than the temperature, T_H, of the wall at $x = L$ (Figure 1). Because of its geometric simplicity, the Fourier problem has been the subject of many studies. One common observation has been that the linear relationship between the heat flux, q, and the local temperature gradient (Fourier's law), given in one dimension by

$$q = -K(T)\frac{dT}{dx}, \tag{1}$$

remains valid even under strongly nonequilibrium (high heat flux) conditions. The validity of Equation 1 for high heat fluxes has been predicted theoretically for gases undergoing Maxwell [13] and BGK [14] interactions, and has also been demonstrated for hard-sphere gases using both molecular dynamics [15,16] and DSMC [9,10,11] numerical simulations. In particular, these studies show that the thermal conductivity observed at high heat flux equals that obtained from CE theory for a nonequilibrium gas in the continuum limit of small heat flux and Knudsen number. CE theory for a hard-sphere gas relates the thermal conductivity to a reference viscosity, μ_{ref}, as [12,11]:

$$K = K_{ref}\left(\frac{T}{T_{ref}}\right)^{1/2} \qquad K_{ref} = \left(\frac{K_\infty}{K_1}\right)\left(\frac{\mu_1}{\mu_\infty}\right)\left(\frac{15}{4}\right)\left(\frac{k_B}{m}\right)\mu_{ref} \tag{2}$$

where K_{ref} and μ_{ref} are evaluated at the reference temperature T_{ref}, $k_B = 1.380658\times10^{-23}$ J/K is the Boltzmann constant, K_∞/K_1 and μ_∞/μ_1 are known CE values, and m is the molecular mass. For a hard-sphere gas, Gallis et al. [11] used CE theory [12] to calculate the infinite-order values $K_\infty/K_1 = 1.025218$ and $\mu_\infty/\mu_1 = 1.016034$.

Gallis et al. [11] performed DSMC simulations that showed that Fourier's law remains valid at high heat fluxes despite the fact that the underlying molecular velocity distribution deviates from CE theory, as measured by the departure of the DSMC-calculated Sonine-polynomial coefficients from the expected CE values. Their work showed that the DSMC method reproduces the CE velocity distribution only in the limit of small local Knudsen numbers (< 0.01); at higher values, the Sonine-polynomial coefficients rapidly diverge from the CE prediction.

DISCRETIZATION ERRORS IN THE DSMC METHOD

Wagner [17] presented a rigorous mathematical proof that numerically resolved (i.e., in the limit of infinite N_c) DSMC simulations provide solutions of the Boltzmann equation. This result suggests that calculations performed with a careful implementation of the DSMC method should agree with theoretical solutions of the Boltzmann equation. Four parameters control numerical error in the DSMC method [1]: the sample size, M_c, the number of simulators per cell, N_c, the time step, Δt, and the cell size, Δx. Bird [1] observed that statistical fluctuations decline with the square root of the sample size and could be reduced (in principle) to any desired level by continuing or repeating the simulation. Hadjiconstantinou et al. [18] recently presented closed-form expressions that relate the statistical error to the sample size in molecular simulation algorithms. In the present study, sufficiently large samples are taken so that statistical errors are reduced to negligible levels.

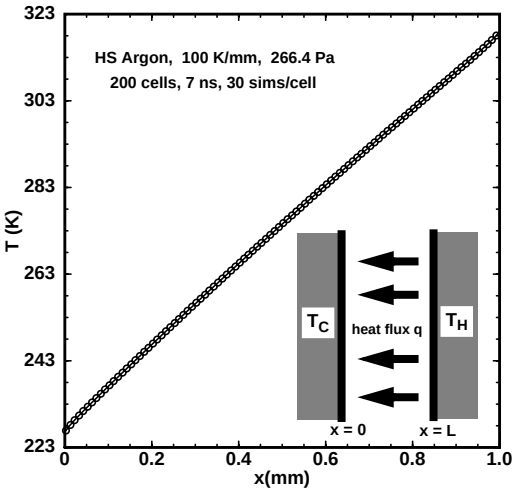

FIGURE 1. Temperature profile for the Fourier geometry (inset).

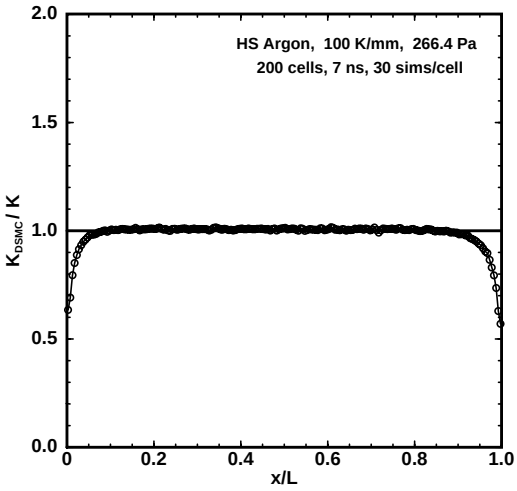

FIGURE 2. Conductivity-ratio profile.

Bird distinguished statistical error from the discretization errors introduced by the three remaining parameters (N_c, Δt, and Δx). Early practitioners of the DSMC method relied on rule-of-thumb guidelines to limit discretization errors. For example, Bird [1] recommended that ~20 or more simulators per cell be used, that cell dimensions should be kept below ~1/3 of the local mean free path, and that the time step should be kept below ~1/4 of the local mean collision time. Later studies have sought to quantify the discretization errors associated with the various numerical approximations. Chen and Boyd [19] analyzed the numerical error inherent in the DSMC method in terms of the sample size and the number of simulators per cell. Their calculations show that the error contains two contributions, a statistical error proportional to $1/\sqrt{M_c}$ and a discretization error proportional to $1/N_c$. Thus, in the limit of vanishing time step and cell size (and infinite sample size), the discretization error in the ratio of the DSMC-calculated thermal conductivity to the CE theoretical value is expected to be of the form:

$$\lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \frac{K_{DSMC}}{K} = 1 + \frac{A}{N_c}, \tag{3}$$

where A is a constant that has not been previously reported in the literature.

Alexander et al. [20] applied Green-Kubo theory to derive explicit expressions for the dependence of hard-sphere gas transport coefficients on cell size. Their expression for the thermal-conductivity ratio, in the limit of vanishing time step and infinite simulators per cell, is:

$$\lim_{\substack{N_c \to \infty \\ \Delta t \to 0}} \frac{K_{DSMC}}{K} = 1 + \frac{32}{225\pi}\left(\frac{\Delta x}{\lambda}\right)^2 = 1 + 0.04527\left(\frac{\Delta x}{\lambda}\right)^2, \tag{4}$$

where Δx is width of the cell in the x-direction, $\lambda = (\sqrt{2}\pi d_{ref}^2 n)^{-1}$ is the hard-sphere gas mean free path, d_{ref} is the molecular diameter, and n is the number density. DSMC calculations [20] of the momentum flux for the Couette-flow problem confirmed the predicted $O(\Delta x^2)$ truncation error and agreed within numerical uncertainty with the Green-Kubo predictions although only two data points were reported in the critical range of interest $\Delta x/\lambda \le 1$.

Hadjiconstantinou [21] applied Green-Kubo theory to derive explicit expressions for the dependence of hard-sphere gas transport coefficients on time step. His expression for the thermal-conductivity ratio, in the limit of vanishing cell size and infinite simulators per cell, is:

$$\lim_{\substack{N_c \to \infty \\ \Delta x \to 0}} \frac{K_{DSMC}}{K} = 1 + \frac{64}{675\pi}\left(\frac{\Delta t}{t_o}\right)^2 = 1 + 0.03018\left(\frac{\Delta t}{t_o}\right)^2, \tag{5}$$

where Δt is the time step, $t_o = \lambda / c_o$ is the hard-sphere mean collision time and $c_o = \sqrt{2k_B T/m}$ is the most probable molecular speed. DSMC simulations for a variety of one-dimensional flows [22] confirmed the predicted $O(\Delta t^2)$ truncation error although only a few data points were reported in the critical range of interest $\Delta t / t_o \le 1$.

DSMC SIMULATIONS

The convergence behavior of the DSMC method is determined for one-dimensional Fourier heat flow of a hard-sphere gas between parallel walls of unequal temperature (see Figure 1 inset). The cold and hot walls are held at 223.15 and 323.15 K, respectively, and are separated by a distance of $L = 1$ mm. All DSMC results below are acquired using a modified version of Bird's one-dimensional code DSMC1 [1,11]. The main modification is the recasting of the code into double precision. In keeping with the spirit of high accuracy, round-off tolerances in several routines were eliminated. The strategy of sampling molecules both before and after the collision stage (move-sample-collide-sample, MSCS) was used [11]. A hard-sphere gas is modeled using argon-like properties ($m = 6.63\times10^{-26}$ kg, $\mu_{ref} = 2.117\times10^{-5}$ Pa · s at $T_{ref} = 273.15$ K) with the VSS collision model ($\omega = 0.5$ and $\alpha = 1$). The molecular diameter is calculated using the Bird strategy [1] as modified by Gallis et al. [11] to account for higher-order CE corrections; the present value for argon-like hard spheres is $d_{ref} = 3.658\times10^{-10}$ m. In all cases, the gas is originally motionless at temperature T_{ref} and pressure $p_{ref} = 266.44$ Pa, and flow transients are allowed to decay for 7 ms before the steady state phase is initiated. The final DSMC-calculated pressure, $p_{DSMC} = 266.9$ Pa, differs slightly from the initial pressure. The final pressure and the reference temperature are used to specify the mean free path and collision time: $\lambda(T_{ref}, p_{DSMC}) = 2.40\times10^{-5}$ m and $t_o(T_{ref}, p_{DSMC}) = 71$ ns. The domain is ~42 mean free paths across, indicating that the Knudsen layers at the walls occupy only a small fraction of the domain.

Time step, cell size, and the number of simulators per cell are systematically varied. The dimensionless time step was selected from the range $0.05 < \Delta t / t_o < 1$, corresponding to physical time steps between 3.5 and 70 ns. The dimensionless cell size was selected from the range $0.05 < \Delta x / \lambda < 0.85$, corresponding to 800 to 50 cells, respectively, across the domain. The number of simulators used in each cell was selected from the range $7 < N_c < 240$. Each simulation is run for ~48 hours on 16 nodes of an IBM Linux cluster, with dual 1.2-GHz P3 processors per node. The parallel implementation of the code speeds the calculations and uses ensemble averaging to provide 95%-confidence intervals for all calculated values. Runs are continued until this uncertainty becomes small compared to the discretization errors, typically requiring $O(10^{10})$ samples per cell. K_{DSMC}/K is calculated for each cell from

$$\frac{K_{DSMC}}{K} = \left(\frac{T_{ref}^{1/2}}{K_{ref}}\right)\left(\frac{|q|}{T^{1/2}}\right)\left(\frac{dT}{dx}\right)^{-1} \tag{6}$$

where q, T, and dT/dx are determined by DSMC. The DSMC-calculated wall heat flux is used for q in Equation 6. Additional numerical error is introduced if the local, cell-based, volume-averaged heat-flux moment is used instead of the wall value. Note that the present MSCS sampling strategy improves the accuracy of volume-averaged flux moments compared to the standard strategy (move-collide-sample, MCS) but has no effect on wall-based values. Thus, the present convergence study applies equally well to either the MCS or MSCS sampling strategies.

The local cell-based value for temperature is used. A profile of a typical DSMC-calculated temperature profile (200 cells, 7-ns time step, 30 simulators per cell) is shown in Figure 1, demonstrating the expected temperature jumps near the walls and a nearly linear profile in the central region of the domain. The temperature gradient is determined from the temperature profile with a central-difference scheme. A conductivity-ratio profile is shown in Figure 2 which has been calculated from Equations 2 and 6 using DSMC simulation results for the same parameter set as in Figure 1. The ratio is observed to lie very close to unity throughout the interior, with Knudsen layers evident near the walls. Some statistical scatter in the points is observed, which is amplified by the need to differentiate the temperature profile. A single measure of the conductivity ratio is found for each calculation by averaging the cell-based conductivity ratios over the central 40% of the domain (well outside the Knudsen layers); this averaging procedure greatly reduces the statistical scatter. The error bars for each data point plotted in Figures 3 and 4 are the 95% confidence interval for each center-averaged value of the conductivity ratio.

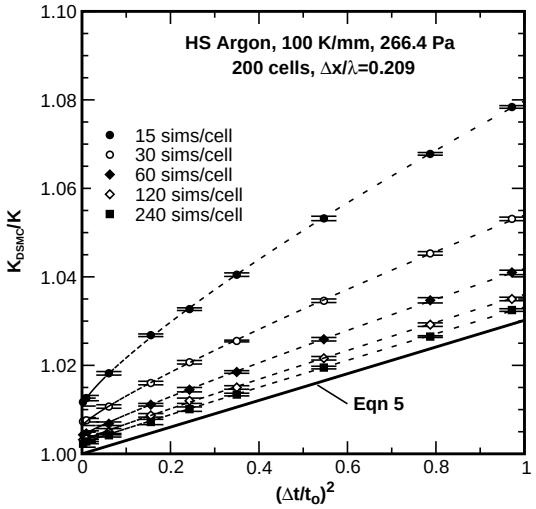

FIGURE 3. Conductivity-ratio dependence on dimensionless time step for various N_c (200 cells).

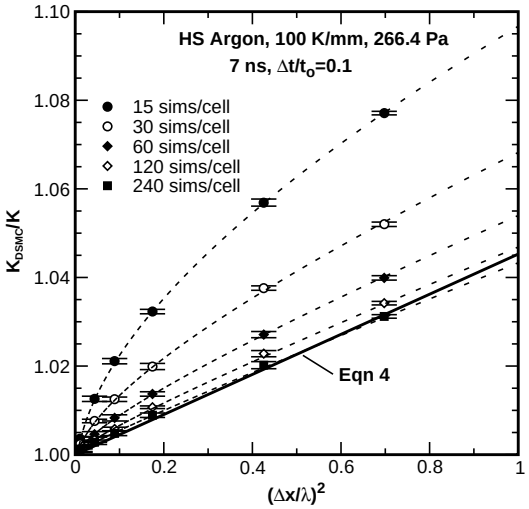

FIGURE 4. Conductivity-ratio dependence on dimensionless cell width for various N_c (Δt = 7 ns).

The convergence behavior of the averaged conductivity ratios is explored systematically with over 200 simulations corresponding to the ranges given above for cell size, time step, and number of simulators. One set of calculations is shown in Figure 3, where the conductivity ratio is plotted against the square of the dimensionless time step for $15 \le N_c \le 240$ and for 200 cells ($\Delta x/\lambda = 0.209$). The theoretical prediction of Equation 5 is also plotted and appears as a straight line. For the largest number of simulators considered, $N_c = 240$, the DSMC calculations lie parallel to, but displaced slightly upward from, the theoretical line. This displacement results from cell-size and finite-simulator discretization errors which have not been eliminated. Although quadratic convergence in time step is approached with increasing simulators, the convergence behavior for fewer than ~60 simulators per cell is clearly not quadratic. Extrapolation of the entire convergence data set to vanishing cell size and infinite N_c gives an estimate for the time-step coefficient, 0.0288, that is in good agreement with the theoretical value, 0.03018.

The convergence behavior of the averaged conductivity ratio with cell size is demonstrated in Figure 4; these calculations were all performed with a fixed time step $\Delta t/t_o = 0.1$ and for $15 \le N_c \le 240$. The theoretical prediction of Equation 4 is also plotted and appears as a straight line. Quadratic convergence in cell size is approached for the largest N_c values tested, although the DSMC calculations are not as parallel to the theoretical result as for the time-step results. Extrapolation of the entire convergence data set to vanishing time step and infinite N_c gives an estimate for the quadratic time-step coefficient, 0.0401, that is in fair agreement with the theoretical value, 0.04527. Again, the convergence behavior with cell size for fewer than ~60 simulators per cell is clearly not quadratic.

A Taylor series expansion in terms of the three parameters was used to perform a least-squares fit of the entire convergence data set. The result of the fitting, shown in both Figures 3 and 4 as dashed lines, agrees extremely well with the DSMC calculations. The statistically-significant, leading terms of the fitting are found to be:

$$\frac{K_{DSMC}}{K} = 1.00016 + 0.0288\left(\frac{\Delta t}{t_o}\right)^2 + 0.0401\left(\frac{\Delta x}{\lambda}\right)^2 - 0.0093\left(\frac{\Delta t}{t_o}\right)\left(\frac{\Delta x}{\lambda}\right)^2 - \frac{0.1474}{N_c} + \frac{1}{N_c}(cross\ terms)\,. \qquad (7)$$

The leading term differs from unity by less than 0.02%, showing that the present DSMC implementation is in remarkable agreement with CE theory. The coefficients of the $1/N_c$ and $\Delta t(\Delta x)^2$ terms have not been previously reported; interestingly, both reduce the conductivity ratio. Higher-order cross terms are also evident.

CONCLUSIONS

A comprehensive study of the numerical convergence behavior of the DSMC method has been completed for the Fourier problem. The study shows that the present implementation of the DSMC method converges to within 0.02% of the CE thermal conductivity in the limit of vanishing cell size and time step with infinite simulators. Quadratic convergence in time step and cell width is observed for $N_c \to \infty$, in good agreement with Green-Kubo theory.

Acknowledgments - This work was performed at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

REFERENCES

[1] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*, Clarendon Press, Oxford (1994).
[2] E. P. Muntz, "Rarefied gas dynamics," *Annu. Rev. Fluid Mech.* **21**, 387-417 (1989).
[3] D. A. Erwin, G. C. Pham-Van-Diep, and E. P. Muntz, "Nonequilibrium gas flow I: A detailed validation of Monte Carlo direct simulation for monatomic gases," *Phys. Fluids A* **3**, 697-705 (1991).
[4] E. Salomons and M. Mareschal, "Usefulness of the Burnett description of strong shock waves," *Phys. Rev. Lett.* **69**, 269-272 (1992).
[5] F. J. Alexander, A. L. Garcia, and B. J. Alder, "Direct simulation Monte Carlo for thin-film bearings," *Phys. Fluids* **6**, 3854-3860 (1994).
[6] M. A. Gallis and J. R. Torczynski, "An improved Reynolds-equation model for gas damping of microbeam motion," *J. MicroElectroMechan. Syst.* **13**, in press (2004).
[7] H. Xue and Q. Fan, "A new analytic solution of the Navier-Stokes equations for microchannel flows," *Micro. Thermophys. Eng.* **4**, 125-143 (2000).
[8] L. S. Pan, G. R. Liu, B. C. Khoo, and B. Song, "A modified direct simulation Monte Carlo method for low-speed microflows," *J. Micromech. Microeng*. **10**, 21-27 (2000).
[9] J. M. Montanero, M. Alaoui, A. Santos, and V. Garzó, "Monte Carlo simulation of the Boltzmann equation for steady Fourier flow," *Phys. Rev. E* **49**, 367-375 (1994).
[10] E. E. Tahiri, M. Tij, and A. Santos, "Monte Carlo simulation of a hard-sphere gas in the planar Fourier flow with a gravity field," *Molec. Phys*. **98**, 239-248 (2000).
[11] M. A. Gallis, J. R. Torczynski, and D. J. Rader, "Molecular gas dynamics observations of Chapman-Enskog behavior and departures therefrom in nonequilibrium gases," *Physical Review E* **69**, paper 042201 (2004).
[12] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, Third Edition, Cambridge University Press, Cambridge, UK (1970).
[13] E. S. Asmolov, N. K. Makashev, and V. I. Nosik, "Heat transfer between plane parallel plates in a gas of Maxwellian molecules," *Sov. Phys. Dokl*. **24**, 892-894 (1979).
[14] A. Santos, J. J. Brey, and V. Garzó, "Kinetic model for steady heat flow," *Phys. Rev. A*. **34**, 5047-5050 (1986).
[15] M. Mareschal, E. Kestemont, F. Baras, E. Clementi, and G. Nicolis, "Nonequilibrium states by molecular dynamics: Transport coefficients in constrained fluids," *Phys. Rev. A*. **35**, 3883-3893 (1987).
[16] P.-J. Clause and M. Mareschal, "Heat transfer in a gas between parallel plates: Moment method and molecular dynamics," *Phys. Rev. A*. **38**, 4241-4252 (1988).
[17] W. Wagner, "A convergence proof for Bird's Direct Simulation Monte Carlo method for the Boltzmann equation," *J. Stat. Phys.* **66**, 1011-1044 (1992).
[18] N. G. Hadjiconstantinou, A. L. Garcia, M. Z. Bazant, and G. He, "Statistical error in particle simulations of hydrodynamic phenomena," *J. Comput. Phys.* **187**, 274-297 (2003).
[19] G. Chen and I. D. Boyd, "Statistical error analysis for the Direct Simulation Monte Carlo technique," *J. Comput. Phys*. **126**: 434-448 (1996).
[20] F. J. Alexander, A. L. Garcia, and B. J. Alder, "Cell size dependence of transport coefficients in stochastic particle algorithms," *Phys. Fluids*, **10**, 1540-1542 (1998); "Erratum," *Phys. Fluids*, **12**, 731 (2000).
[21] N. G. Hadjiconstantinou, "Analysis of discretization in the direct simulation Monte Carlo," *Phys. Fluids*, **12**, 2634-2638 (2000).
[22] A. L. Garcia and W. Wagner, "Time step truncation error in direct simulation Monte Carlo," *Phys. Fluids*, **12**, 2621-2633 (2000).